Critical Properties in Photoemmision Spectra for One Dimensional Orbitally Degenerate Mott Insulator

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Critical properties in photoemission spectra for the onedimensional Mott insulator with orbital degeneracy are studied by exploiting the integrable t-J model, which is a supersymmetric generalization of the $\mathrm{SU}(n)$ degenerate spin model. We discuss the critical properties for the holon dispersion as well as the spinon dispersions, by applying the conformal field theory analysis to the exact finite-size energy spectrum. We study the effect of orbital-splitting on the spectra by evaluating the momentum-dependent critical exponents.

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I. INTRODUCTION

The recent experiments on the angular resolved photoemission for one-dimensional (1D) correlated electron systems [1–7] have revealed some striking properties inherent in 1D systems, such as the spin-charge separation. In particular, the photoemission experiments [5-7] for the Mott insulator compound SrCuO₂, Sr₂CuO₃ and NaV₂O₅ have clarified characteristic properties of a single hole doped in the 1D Mott insulator. So far, extensive theoretical studies on spectral functions for 1D correlated systems have been done numerically [8–15] and analytically. [16–22] Among others, it has been recently shown [16,19,20] that the dynamical spectral functions for the 1D Mott insulator still show the power-law singularity at threshold energies, characterizing the critical properties of a doped hole in the 1D Mott insulator. For example, Sorella and Parola [19] have addressed this problem based on the conformal field theory (CFT) analysis of the supersymmetric t-J model. Also, such an analysis has been extended to the anisotropic t-J model with either the spin gap or the charge gap. [22]

In some compounds of the Mott insulator, such as Mn oxides, it is known that the orbital degrees of freedom as well as the spin degrees of freedom play an important role. [23] These hot topics on the Mott insulator have stimulated the theoretical studies on the orbitally degenerate Hubbard model and the related correlated electron systems. As a first step to explore such orbital effects more precisely, the 1D version of the degenerate Hubbard model in the strong coupling regime has been extensively studied. [24–26]

Motivated by the above investigations, we study the critical properties in photoemission spectra for the 1D

Mott insulator with orbital degeneracy. For this purpose, we consider the 1D SU(n) spin model as a Mott insulator in the strong coupling regime. Doping a hole into the model is incorporated by exploiting the integrable t-J model, which is a supersymmetric generalization of the SU(n) spin model. [27] We shall discuss the critical properties in photoemission spectra for the holon as well as spinon dispersions, based on the CFT analysis of the above integrable model.

This paper is organized as follows. In § 2 we introduce the model, and present the calculational detail which is necessary to study the low-energy critical properties. Our main strategy is the finite-size scaling technique applied to the energy spectrum, in which we should properly take into account a final-state interaction between the massless spinons and the massive holon created by photoemission. Then in § 3 we derive the spectral functions and their critical exponents based on the CFT analysis. We discuss photoemission spectra for the massive holon dispersion for SU(n) symmetric case, and then applying a similar technique, we also study a power-law singularity for the (n-1) spinon dispersions. We discuss the effect of orbital splitting by exploiting the SU(4) spin model with two-band structure, for which we obtain the momentum-dependent critical exponents for the photoemission spectra. Brief summary is given in § 4.

II. CONFORMAL PROPERTIES OF ORBITALLY DEGENERATE MOTT INSULATOR WITH A HOLE

A. Model and basic equations

Let us start with the ordinary Hubbard model with on-site Coulomb interaction and Hund coupling, which possesses L-orbitals and spins $\sigma = \uparrow, \downarrow$. In the case of the strong on-site Coulomb interaction in the insulating phase, the model is generally reduced to the Kugel-Khomskii type model. [28] If we neglect the Hund coupling for simplicity, the symmetry of the system is enhanced and the resulting model becomes the SU(2L) exchange model, for which 2L indices specify both of the orbital and spin degrees of freedom. [24,25] We study this exchange model as the spin and orbital parts of the Mott insulator. Doping a hole into the exchange model induces a kinetic term, which should be taken into account to discuss the photoemission spectrum. To this end, we

use the supersymmetric t-J model for which the electron hopping t is assumed to be equal to the exchange coupling J. The advantage to use this model is that it allows us to treat various quantities exactly. Let us now write down the Hamiltonian for the multi-orbital t-J model,

$$\mathcal{H} = -t \sum_{i} \sum_{\sigma,m} (c_{i,\sigma}^{m\dagger} c_{i+1,\sigma}^{m} + c_{i+1,\sigma}^{m\dagger} c_{i,\sigma}^{m})$$

$$+ J \sum_{i} \sum_{\sigma,\sigma'} \sum_{m,m'} (c_{i,\sigma}^{m\dagger} c_{i,\sigma'}^{m'} c_{i+1,\sigma'}^{m'\dagger} c_{i+1,\sigma}^{m} - n_{i} n_{i+1})$$

$$- \sum_{m} \sum_{i} \Delta_{m} (n_{i}^{(m)} - n_{i}^{(m+1)}),$$
(1)

where $c_{i,\sigma}^{m\dagger}$ is the creation operator for electrons. It is implicitly assumed that multiple occupation of each site is forbidden. Each orbital, which is labeled by $m(=1,2,\cdots,L)$ and is energetically separated from each other by the orbital-splitting Δ_m , has two spin states $(\sigma=\uparrow,\downarrow)$. At the supersymmetric point t=J which we are interested in, the model is exactly solvable. [27,29]

In the following, we exactly analyze the low-energy properties of the model in the insulating state (one electron for every site) with one hole, since one electron is emitted from the system in photoemission experiments. To this end, we first write down the relevant Bethe equations for the model (1), which describe excitations when one electron is emitted from the insulating system. For convenience, we introduce the number n=2L and the index $\mu(=1,\cdots,n-1)$ which specifies the spin as well as orbital excitations on equal footing. The Bethe equations consist of (n-1) kinds of rapidities $\lambda_{\alpha}^{(\mu)}$ for spin and orbital degrees of freedom, [27]

$$-N\Theta_{2}(\lambda_{\alpha}^{(\mu)})\delta_{\mu 1} + 2\pi I_{\alpha}^{(\mu)} = \sum_{\nu=1}^{n-1} \sum_{\beta=1}^{M_{\mu}} \Theta_{\mu\nu} (\lambda_{\alpha}^{(\mu)} - \lambda_{\beta}^{(\nu)}) + \Theta_{2}(\lambda_{\alpha}^{(\mu)} - q)\delta_{\mu n-1} \quad 1 \le \alpha \le M_{\mu},$$
(2)

where $\Theta_{\mu\nu} = -\Theta_1 \delta_{\mu\nu} + \Theta_2(\delta_{\mu\nu+1} + \delta_{\mu+1\nu})$, and $\Theta_n(\lambda) = 2 \tan^{-1}(n\lambda)$. Here we have introduced the quantity, $M_{\mu} = \sum_{\gamma=\mu+1}^{n+1} N_{\gamma}$, in (2), where N_{γ} is the number of particles which belong to the type γ ($\gamma = 1, \dots, n+1$).

It is to be noticed here that there exists an impurity $term\ \Theta_2(\lambda_{\alpha}^{(\mu)}-q)\delta_{\mu n-1}$ in the above Bethe equations. This is the term which indeed describes a scattering due to the hole created in photoemission, where a charge rapidity q specifies the momentum of the created hole. In this sense, this scattering term due to the created hole can be regarded as a final-state interaction caused by the photoemission. For simplicity, in this paper we shall refer to (n-1) massless excitations as spinons while the above charge excitation as holon. Needless to say, the holon excitation is massive because of the existence of the Mott-Hubbard gap. We will see that although massive holon excitation does not directly enter in the low

energy physics, it controls the critical behavior of massless spin excitations via a final-state interaction.

Finally we note that each quantum number $I_{\alpha}^{(\mu)}$ is subject to the selection rule (gluing condition for electrons),

$$I_{\alpha}^{(\mu)} = -\frac{1}{2}(M_{\mu-1} - M_{\mu} + M_{\mu+1}) + M_{\mu+1}\delta_{\mu 1} \mod 1,$$
(3)

which plays an essential role when we read the critical exponents from the finite-size spectrum.

B. Finite-size corrections

In order to apply the methods developed in CFT, [30] we now evaluate the finite-size corrections to the ground-state energy and the excitation energy. [31,32] The key point in our case is to take into account a final-state interaction properly, i.e. the scattering phase shift due to the massive holon. Since the calculation of the spectrum is performed in a standard way, [33,19] we briefly summarize the outline of the calculation in the following. We also mention that the present calculation has a close relationship to that for 1D solvable systems with a impurity or boundaries. [34–40]

The total energy and the total momentum are given in terms of the rapidities,

$$E = \sum_{\alpha=1}^{n} \sum_{j=1}^{M_{\alpha}} \varepsilon_{\alpha}^{0}(\lambda_{j}^{\alpha}), \quad P = \sum_{\alpha=1}^{n} \sum_{j=1}^{M_{\alpha}} p_{\alpha}^{0}(\lambda_{j}^{\alpha}). \tag{4}$$

According to the Euler-Maclaurin formula, we can obtain the finite-size corrections to the ground-state energy in a standard form,

$$E_0 = N\epsilon_0 - \sum_{\alpha=1}^{n-1} \frac{\pi v_\alpha}{6N},\tag{5}$$

where $N\epsilon_0$ is the ground-state energy in the thermodynamic limit. Here v_{α} is the velocity of massless spinons labeled by α ,

$$v_{\alpha} = \frac{\varepsilon_{\alpha}^{'}(\lambda_{\alpha})}{2\pi\sigma_{\infty\alpha}(\lambda_{\alpha})} \big|_{\lambda_{\alpha} = \lambda_{\alpha}^{0}} , \qquad (6)$$

where

$$\begin{split} \varepsilon_{\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm}) &= \varepsilon_{\alpha}^{0}(\lambda_{\alpha}) \\ &+ \sum_{\gamma=1}^{n-1} \int_{\lambda_{\gamma}^{-}}^{\lambda_{\gamma}^{+}} K_{\alpha\gamma}(\lambda_{\alpha} - \lambda_{\gamma}^{'}) \varepsilon_{\gamma}(\lambda_{\gamma}^{'}|\lambda_{\nu}^{\pm}) \mathrm{d}\lambda_{\gamma}^{'}, \\ \sigma_{\infty\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm}) &= \sigma_{\infty\alpha}^{0}(\lambda_{\alpha}) \\ &+ \sum_{\gamma=1}^{n-1} \int_{\lambda_{\gamma}^{-}}^{\lambda_{\gamma}^{+}} K_{\alpha\gamma}(\lambda_{\alpha} - \lambda_{\gamma}^{'}) \sigma_{\infty\gamma}(\lambda_{\gamma}^{'}|\lambda_{\nu}^{\pm}) \mathrm{d}\lambda_{\gamma}^{'}, \end{split}$$

with $\sigma_{\infty\alpha}^0(\lambda_{\alpha}) = \frac{1}{2\pi}\Theta_2'(\lambda_{\alpha})\delta_{\alpha 1}$ and $K_{\alpha\gamma}(\lambda) = \frac{1}{2\pi}\Theta_{\alpha\gamma}'(\lambda)$. The quantity $\varepsilon_{\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm})$ is called the dressed energy, and the "Fermi points" λ_{α}^{\pm} of massless spinons are determined by the condition, $\varepsilon_{\alpha}(\lambda_{\alpha}^{\pm}|\lambda_{\nu}^{\pm}) = 0$. As should be expected, the expression for the ground-state energy (5) is typical for (n-1) independent c=1 Gaussian CFTs, which indeed coincides with the known formula for the SU(n) spin chain. [41,42] So, one cannot see the effect of the holon at this stage.

Let us next analyze the excited energy $\Delta E = E - E_0$ and the associated momentum $\Delta P = P - P_0$ when a hole is created by the photoemission. Because of spin-charge decoupling, the excited energy and momentum are naturally written as a sum of a holon term and a spinon term,

$$\Delta E = \Delta \varepsilon_c(q) + \Delta \varepsilon_s(\lambda_{\nu}^{\pm}),$$

$$\Delta P = \Delta p_c(q) + \Delta p_s(\lambda_{\nu}^{\pm}),$$
(7)

where $\Delta \varepsilon_c(q)$ ($\Delta p_c(q)$) is the excitation energy (momentum) of a massive holon while $\Delta \varepsilon_s(\lambda_{\nu}^{\pm})$ ($\Delta p_s(\lambda_{\nu}^{\pm})$) are those of (n-1) types of spinons.

Since the quantities for holon, $\Delta \varepsilon_c(q)$ and $\Delta p_c(q)$, can be easily calculated, which give the holon dispersion, we shall concentrate on the finite-size corrections in the massless spin sector, $\Delta \varepsilon_s(\lambda_{\nu}^{\pm}), \Delta p_s(\lambda_{\nu}^{\pm})$, by properly treating a final-state interaction. The energy for the spin sector is given by

$$\varepsilon_s(\lambda_{\nu}^{\pm}) = N \sum_{\alpha=1}^{n-1} \int_{\lambda_{\alpha}^{-}}^{\lambda_{\alpha}^{+}} \sigma_{\alpha}^{0}(\lambda_{\alpha}) \varepsilon_{\alpha}(\lambda_{\alpha} | \lambda_{\nu}^{\pm}) d\lambda_{\alpha}, \tag{8}$$

where $\sigma_{\alpha}^{0}(\lambda_{\alpha}) = \sigma_{\infty,\alpha}^{0}(\lambda_{\alpha}) + \frac{1}{N}\sigma_{c,\alpha}^{0}(\lambda_{\alpha})$ and $\sigma_{c,\alpha}^{0}(\lambda_{\alpha}) = \frac{1}{2\pi}\Theta_{2}^{'}(\lambda_{\alpha} - q)\delta_{\alpha n - 1}$. Let us expand $\varepsilon_{s}(\lambda_{\nu}^{\pm})$ around the ground-state energy $N\varepsilon_{0} = \varepsilon_{s}(\pm\lambda_{\nu}^{0})$,

$$\Delta \varepsilon_{s}(\lambda_{\nu}^{\pm}) = \frac{1}{2} \sum_{\alpha=1}^{n-1} \left\{ \frac{\partial^{2} \varepsilon_{s}}{\partial \lambda_{\alpha}^{+2}} \left|_{\lambda_{\alpha}^{+} = \lambda_{\alpha}^{0}} \left(\lambda_{\alpha}^{+} - \lambda_{\alpha}^{0}\right)^{2} + \frac{\partial^{2} \varepsilon_{s}}{\partial \lambda_{\alpha}^{-2}} \left|_{\lambda_{\alpha}^{-} = -\lambda_{\alpha}^{0}} \left(\lambda_{\alpha}^{-} + \lambda_{\alpha}^{0}\right)^{2} \right\} \right\}.$$

$$(9)$$

Recall here that the deviation of the Fermi points, $\lambda_{\alpha}^{+} - \lambda_{\alpha}^{0}$ and $\lambda_{\alpha}^{-} + \lambda_{\alpha}^{0}$, should be related to the change of the particle number and also the current induced in the system. First, we note that the number of particles M_{α}^{0} and the current D_{α}^{0} for each spinon in the ground state is given by

$$\begin{split} \frac{M_{\alpha}^{0}}{N} &= \int_{-\lambda_{\alpha}^{0}}^{+\lambda_{\alpha}^{0}} \sigma_{\infty\alpha}(\lambda_{\alpha}| \pm \lambda_{\nu}^{0}), \\ \frac{D_{\alpha}^{0}}{N} &= \frac{1}{2} \left(\frac{1}{2\pi} z_{\infty\alpha}(+\infty) + \frac{1}{2\pi} z_{\infty\alpha}(-\infty) \right) \\ &- \frac{1}{2} \left(\int_{+\lambda_{\alpha}^{0}}^{\infty} \sigma_{\infty\alpha}(\lambda_{\alpha}| \pm \lambda_{\nu}^{0}) - \int_{-\infty}^{-\lambda_{\alpha}^{0}} \sigma_{\infty\alpha}(\lambda_{\alpha}| \pm \lambda_{\nu}^{0}) \right), \end{split}$$

where

$$z_{\infty\alpha}(\lambda_{\alpha}) = \Theta_{2}(\lambda_{\alpha})\delta_{\alpha 1} + \sum_{\gamma=1}^{n-1} \int_{-\lambda_{\alpha}^{0}}^{+\lambda_{\alpha}^{0}} \Theta_{\alpha\gamma}(\lambda_{\alpha} - \lambda_{\gamma}^{'})\sigma_{\infty\gamma}(\lambda_{\gamma}^{'}| \pm \lambda_{\nu}^{0})d\lambda_{\gamma}^{'}.$$

On the other hand, if one electron is emitted from the system the above relations should read

$$\begin{split} \frac{M_{\alpha}^{0}+1}{N} &= \int_{\lambda_{\alpha}^{-}}^{\lambda_{\alpha}^{+}} \sigma_{\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm}) \\ &= \int_{\lambda_{\alpha}^{-}}^{\lambda_{\alpha}^{+}} \left(\sigma_{\infty\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm}) + \frac{1}{N}\sigma_{c,\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm})\right), \\ \frac{D_{\alpha}^{0}+1/2\delta_{\alpha,1}}{N} &= \frac{1}{2} \left(\frac{1}{2\pi}z_{\alpha}(+\infty) + \frac{1}{2\pi}z_{\alpha}(-\infty)\right) \\ &\quad - \frac{1}{2} \left(\int_{\lambda_{\alpha}^{+}}^{\infty} \sigma_{\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm}) - \int_{-\infty}^{\lambda_{\alpha}^{-}} \sigma_{\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm})\right), \end{split}$$

where

$$z_{\alpha}(\lambda_{\alpha}) = \Theta_{2}(\lambda_{\alpha})\delta_{\alpha 1} + \frac{1}{N}\Theta_{2}(\lambda_{\alpha} - q)\delta_{\alpha n - 1} + \sum_{\gamma = 1}^{n - 1} \int_{\lambda_{\alpha}^{-}}^{\lambda_{\alpha}^{+}} \Theta_{\alpha \gamma}(\lambda_{\alpha} - \lambda_{\gamma}^{'})\sigma_{\gamma}(\lambda_{\gamma}^{'}|\lambda_{\nu}^{\pm})d\lambda_{\gamma}^{'}.$$

Therefore, one can find that the change in the particle number $\Delta M_{\alpha} = M_{\alpha} - M_{\alpha}^{0}$ and the induced current $\Delta D_{\alpha} = D_{\alpha} - D_{\alpha}^{0}$ satisfy

$$\frac{\Delta M_{\alpha} + 1 - n_{c,\alpha}}{N} = \sum_{\beta=1}^{n-1} \xi_{\alpha\beta}(\lambda_{\beta}^{0}) \sigma_{\infty\beta}(\lambda_{\beta}^{0})(\lambda_{\beta}^{+} - \lambda_{\beta}^{0})
- \xi_{\alpha\beta}(-\lambda_{\beta}^{0}) \sigma_{\infty\beta}(-\lambda_{\beta}^{0})(\lambda_{\beta}^{-} + \lambda_{\beta}^{0}),
\frac{\Delta D_{\alpha} + 1/2\delta_{\alpha,1} - d_{c,\alpha}}{N} = \sum_{\beta=1}^{n-1} z_{\alpha\beta}(\lambda_{\beta}^{0}) \sigma_{\infty\beta}(\lambda_{\beta}^{0})(\lambda_{\beta}^{+} - \lambda_{\beta}^{0})
+ z_{\alpha\beta}(-\lambda_{\beta}^{0}) \sigma_{\infty\beta}(-\lambda_{\beta}^{0})(\lambda_{\beta}^{-} + \lambda_{\beta}^{0}),$$
(10)

where we have neglected terms of $O(1/N^2)$. We can see from (3) that the quantum numbers ΔM_{α} and ΔD_{α} are subject to the selection rule (gluing condition)

$$\Delta D_{\mu} = -\frac{1}{2}(\Delta M_{\mu-1} + \Delta M_{\mu+1}) + \Delta M_{\mu+1}\delta_{\mu 1} \mod 1.$$
(11)

The quantities $\xi_{\alpha\beta} = \xi_{\alpha\beta}(\lambda_{\beta}^0 | \pm \lambda_{\nu}^0)$ are the so called dressed charges which are given by the solution to the integral equations [42]

$$\xi_{\alpha\beta}(\lambda_{\beta}|\pm\lambda_{\nu}^{0}) = \delta_{\alpha\beta} + \sum_{\gamma=1}^{n-1} \int_{-\lambda_{\gamma}^{0}}^{+\lambda_{\gamma}^{0}} \xi_{\alpha\gamma}(\lambda_{\gamma}^{'}|\pm\lambda_{\nu}^{0}) K_{\gamma\beta}(\lambda_{\gamma}^{'}-\lambda_{\beta}) d\lambda_{\gamma}^{'}.$$

Note that the quantities of $z_{\alpha\beta}(\lambda_{\beta}^0|\pm\lambda_{\nu}^0)$ introduced in (10) are related to the dressed charges: $2\sum_{\beta} z_{\alpha\beta}\xi_{\beta\gamma} = \delta_{\alpha\gamma}$.

A remarkable point in (10) is that two kinds of phase shifts $n_{c,\alpha}$ and $d_{c,\alpha}$, which are the key quantities to control the anomalous low-energy properties, enter in (10). These phase shifts, which are caused by a final-state interaction between spinons and the created holon, are explicitly obtained as

$$\begin{split} n_{c,\alpha} &= \int_{-\lambda_{\alpha}^{0}}^{+\lambda_{\alpha}^{0}} \sigma_{c,\alpha}(\lambda_{\alpha}| \pm \lambda_{\nu}^{0}), \\ d_{c,\alpha} &= \frac{1}{2} \left(\frac{1}{2\pi} z_{c,\alpha}(\infty) + \frac{1}{2\pi} z_{c,\alpha}(-\infty) \right) \\ &- \frac{1}{2} \left(\int_{+\lambda_{\alpha}^{0}}^{\infty} \sigma_{c,\alpha}(\lambda_{\alpha}| \pm \lambda_{\nu}^{0}) - \int_{-\infty}^{-\lambda_{\alpha}^{0}} \sigma_{c,\alpha}(\lambda_{\alpha}| \pm \lambda_{\nu}^{0}) \right), \end{split}$$

where

$$\begin{split} \sigma_{c,\alpha}(\lambda_{\alpha}|\lambda_{\nu}^{\pm}) &= \sigma_{c,\alpha}^{0}(\lambda_{\alpha}) \\ &+ \sum_{\gamma=1}^{n-1} \int_{-\lambda_{\gamma}^{0}}^{+\lambda_{\gamma}^{0}} K_{\alpha\gamma}(\lambda_{\alpha} - \lambda_{\gamma}^{'}) \sigma_{c,\gamma}(\lambda_{\gamma}^{'}| \pm \lambda_{\nu}) \mathrm{d}\lambda_{\gamma}^{'}, \\ z_{c,\alpha}(\lambda_{\alpha}) &= \Theta_{2}(\lambda_{\alpha} - q) \delta_{\alpha n - 1} \\ &+ \sum_{\gamma=1}^{n-1} \int_{-\lambda_{\alpha}^{0}}^{+\lambda_{\alpha}^{0}} \Theta_{\alpha\gamma}(\lambda_{\alpha} - \lambda_{\gamma}^{'}) \sigma_{c,\gamma}(\lambda_{\gamma}^{'}| \pm \lambda_{\nu}^{0}) \mathrm{d}\lambda_{\gamma}^{'}. \end{split}$$

Combining the above expressions, we end up with the excitation energy,

$$\Delta \varepsilon_s = \sum_{\alpha=1}^{n-1} \frac{2\pi v_{\alpha}}{N} \{ \frac{1}{4} (\xi^{-1} \mathbf{n})_{\alpha}^2 + (\xi^T \mathbf{d})_{\alpha}^2 + N_{\alpha}^+ + N_{\alpha}^- \},$$

where we have added particle-hole excitations specified by the quantum numbers N_{α}^{+} and N_{α}^{-} . Here we have introduced the notation

$$(\xi)_{\alpha\beta} = \xi_{\alpha\beta}, \quad (\mathbf{n})_{\alpha} = \Delta M_{\alpha} + 1 - n_{c,\alpha},$$

$$(\mathbf{d})_{\alpha} = \Delta D_{\alpha} + \frac{1}{2} \delta_{\alpha,1} - d_{c,\alpha}.$$
(12)

Performing a similar manipulation, the excited momentum Δp_s is also obtained as

$$\Delta p_{s} = 2\pi \sum_{\alpha=1}^{n-1} Q_{F,\alpha}(\mathbf{d})_{\alpha} + \frac{2\pi}{N} \sum_{\alpha=1}^{n-1} \{ (\mathbf{n})_{\alpha} + (\mathbf{d})_{\alpha} + N_{\alpha}^{+} - N_{\alpha}^{-} \}.$$
 (13)

This completes the calculation of the finite-size corrections.

C. Conformal dimensions

According to the finite-size scaling in CFT, conformal dimensions Δ_{α}^{\pm} of α -type spinons are read from the universal 1/N corrections to the excitation energy $\Delta \varepsilon_s$ and momentum Δp_s , which are given by

$$\Delta_{\alpha}^{+} + \Delta_{\alpha}^{-} = \frac{1}{4} (\xi^{-1} \mathbf{n})_{\alpha}^{2} + (\xi^{T} \mathbf{d})_{\alpha}^{2} + N_{\alpha}^{+} + N_{\alpha}^{-},$$

$$\Delta_{\alpha}^{+} - \Delta_{\alpha}^{-} = (\mathbf{n})_{\alpha} + (\mathbf{d})_{\alpha} + N_{\alpha}^{+} - N_{\alpha}^{-}.$$
(14)

So, they are reduced to

$$\Delta_{\alpha}^{\pm} = \frac{1}{2} \left(\frac{1}{2} \xi^{-1} \mathbf{n} \pm \xi^{T} \mathbf{d} \right)_{\alpha}^{2} \pm N_{\alpha}^{\pm}. \tag{15}$$

Although conformal dimensions Δ_{α}^{\pm} for massless spinons are typical for c=1 CFTs, [43,44] the massive holon also contributes to Δ_{α}^{\pm} via the phase shifts $n_{c,\alpha}(q)$ and $d_{c,\alpha}(q)$. In this sense, (15) is classified as shifted c=1 CFTs, whose fixed point is different even from that of the static impurity problem, as pointed out by Sorella and Parola. [19] This fixed point indeed belongs to that of mobile-impurity class in 1D quantum systems, [45] for which two kinds of phase shifts play a crucial role.

III. ONE-PARTICLE GREEN FUNCTION AND PHOTOEMISSION SPECTRA

A. Critical properties for holon dispersion

Having classified low-energy properties by CFT, we are now ready to investigate the critical properties of the one-electron Green function at absolute zero, which is defined by

$$G_{\beta}(x,t) = i \sum_{q} \theta(-t) e^{i\Delta\varepsilon_{c}t - i\Delta p_{c}x}$$

$$\times \sum_{N,\bar{N}=0}^{\infty} \langle 0|\psi^{\dagger}(0)|N,\bar{N}\rangle \langle N,\bar{N}|\psi(0)|0\rangle e^{i\Delta\varepsilon_{s}t - i\Delta p_{s}x},$$
(16)

for $\beta=0,\cdots,n-1$, where |0> represents the ground state. Exploiting finite-size scaling in CFT, we can write down its asymptotic form as

$$\sum_{N,\bar{N}=0}^{\infty} <0|\psi^{\dagger}(0)|N,\bar{N}> < N,\bar{N}|\psi(0)|0> \mathrm{e}^{\mathrm{i}\Delta\varepsilon_{s}t-\mathrm{i}\Delta p_{s}x}$$

$$\to \prod_{\alpha=1}^{n-1} \frac{e^{-i2\pi Q_{F,\alpha}(\mathbf{d})_{\alpha}x}}{(x-v_{\alpha}t)^{2\Delta_{\alpha}^{+}}(x+v_{\alpha}t)^{2\Delta_{\alpha}^{-}}},$$

where Δ_{α}^{\pm} are conformal dimensions which are related to the scaling dimensions x_{β} ,

$$x_{\beta} = \sum_{\alpha=1}^{n-1} (\Delta_{\alpha}^{+} + \Delta_{\alpha}^{-})$$
$$= \frac{1}{4} \mathbf{n}^{T} (\xi^{-1})^{T} (\xi^{-1}) \mathbf{n} + \mathbf{d}^{T} \xi \xi^{T} \mathbf{d}.$$
(17)

The asymptotic form of the spectral function $A_{\beta}(k, w)$ around the holon dispersion is given via the Fourier transformation as

$$A_{\beta}(k,\omega) = \frac{1}{\pi} \operatorname{Im} G_{\beta}(k,\omega) \sim (\omega - \omega_c(k-Q))^{X_{\beta}(k)}$$
(18)

with the critical exponent

$$X_{\beta}(k) = 2x_{\beta} - 1,\tag{19}$$

where the energy $\omega_c(k-Q) = \Delta \varepsilon_c(q)$ and the momentum $Q = 2\pi \sum_{\alpha=1}^{n-1} Q_{F,\alpha}(\mathbf{d})_{\alpha}$ feature the dispersion of holon. We can see that the singularity in the spectral function which occurs at frequencies determined by the holon dispersion is governed by the critical exponent $X_{\beta}(k)$ for spinons. [19] Namely, this exponent reflects the infrared divergence properties of spinons, which also includes the phase shifts $n_{c,\alpha}, d_{c,\alpha}$ caused by a final state interaction. These two phase shifts usually depend on a rapidity of the holon excitation, giving rise to the momentum dependent critical exponents in generic cases.

Now our problem is to read the correct scaling dimensions by appropriately choosing a set of quantum numbers, to describe the critical behavior of photoemission spectrum. The key to choose the quantum numbers is the selection rule given in (11). Since we are now considering the situation that one electron is emitted from the system, one holon and one spinon should be removed. This gives the guideline to set the quantum numbers. Suppose that an electron of β -type is emitted from the system, then we rewrite the quantum numbers as, $\Delta M_{\alpha} \to (\Delta \mathbf{M}^{\beta})_{\alpha}$ and $\Delta D_{\alpha} \to (\Delta \mathbf{D}^{\beta})_{\alpha}$, which can be chosen as

$$(\Delta \mathbf{M}^{\beta})_{\alpha} = -1 \quad (0 \le \alpha \le \beta), \quad 0 \quad (\beta < \alpha \le n - 1),$$

$$(\Delta \mathbf{D}^{\beta})_{\alpha} = -\frac{1}{2}\delta_{\alpha 1} + \frac{1}{2}\delta_{\alpha \beta} - \frac{1}{2}\delta_{\alpha \beta + 1}.$$
 (20)

Let us first consider the $\mathrm{SU}(n)$ case without orbital splitting. In this case, the $(n-1)\times(n-1)$ dressed charge matrix is easily evaluated as,

$$(\xi^{-1})^T(\xi^{-1}) = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots \\ & & -1 & 2 \end{pmatrix}, \tag{21}$$

which is nothing but the Cartan matrix for SU(n) Lie algebra. [41] Note that $\xi \xi^T$ is given by the inverse of the above matrix. By substituting the quantum numbers, we consequently obtain the corresponding scaling dimension,

$$x_{\beta}(k) = \frac{1}{2}(1 - \frac{1}{n}) \tag{22}$$

for $\beta = 0, 1, \dots, n-1$. Thus the critical exponent for the holon dispersion is $X_{\beta} = -1/n$. Therefore, if the orbital degeneracy becomes large, the singular property is expected to become weaker. In the special case of n = 2, this exponent was already obtained. [19,20] Note that the above exponent depends neither on the spin and

orbital indices nor on the momentum. This simple result follows from that SU(n) symmetry holds exactly in the case without orbital splitting.

We now wish to discuss the effect of orbital splitting on the critical exponents. In the following, we concentrate on the specific case of two orbital (n=2L=4) to see our discussions more clearly, [46] since the generalization to $\mathrm{SU}(n)$ can be done straightforwardly. We note that such an orbital splitting may come from the crystalline field effects. In the $\mathrm{SU}(4)$ case, there appear three types of spinons, the Fermi points of which are: λ_2^0 is finite, which is due to $\mathrm{U}(1)$ symmetry induced by an orbital splitting $\Delta_1 = \Delta$, while λ_1^0 and λ_3^0 are infinite, reflecting that each spinon excitation in the same orbital still has $\mathrm{SU}(2)$ symmetry. Accordingly, we have the matrix, [46]

$$(\xi^{-1})^{T}(\xi^{-1}) = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 1 + \frac{1}{\xi_{\Delta}^{2}} & -1 \\ 0 & -1 & 2 \end{pmatrix},$$

$$\xi \xi^{T} = \begin{pmatrix} 1 + \frac{\xi_{\Delta}^{2}}{2} & \xi_{\Delta}^{2} & \frac{\xi_{\Delta}^{2}}{2} \\ \xi_{\Delta}^{2} & 2\xi_{\Delta}^{2} & \xi_{\Delta}^{2} \\ \frac{\xi_{\Delta}^{2}}{2} & \xi_{\Delta}^{2} & 1 + \frac{\xi_{\Delta}^{2}}{2} \end{pmatrix}.$$
 (23)

The dressed charge $\xi_{\Delta} \equiv \xi_{\Delta}(\lambda_2^0)$ for U(1) part is given by the integral equation,

$$\xi_{\Delta}(\lambda|\pm\lambda_{2}^{0}) = 1 + \int_{-\lambda_{2}^{0}}^{+\lambda_{2}^{0}} G(\lambda-\lambda')\xi_{\Delta}(\lambda'|\pm\lambda_{2}^{0}), \quad (24)$$

where the integral kernel $G(\lambda)$ is

$$G(\lambda) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \frac{1 - \mathrm{e}^{|k|}}{1 + \mathrm{e}^{|k|}} \mathrm{e}^{ik\lambda}.$$
 (25)

As mentioned above, this system has SU(4) symmetry in a vanishing orbital-splitting, so that $\xi_{\Delta} \to 1$ and $(\xi^{-1})^T(\xi^{-1})$ becomes SU(4) Cartan matrix.

We rewrite the scaling dimensions by using (23),

$$x_0 = x_1 = \frac{1}{4} + \frac{1}{4\xi_{\Delta}^2} (1 - n_c)^2 + \xi_{\Delta}^2 (-\frac{1}{4} - d_c)^2,$$

$$x_2 = x_3 = \frac{1}{4} + \frac{1}{4\xi_{\Delta}^2} (-n_c)^2 + \xi_{\Delta}^2 (\frac{1}{4} - d_c)^2,$$
 (26)

where,

$$\begin{split} n_c &= \int_{-\lambda_2^0}^{+\lambda_2^0} \sigma_c(\lambda|\pm\lambda_2^0) \\ d_c &= \frac{1}{2} \left(\int_{-\infty}^{-\lambda_2^0} \sigma_c(\lambda|\pm\lambda_2^0) - \int_{+\lambda_2^0}^{\infty} \sigma_c(\lambda|\pm\lambda_2^0) \right), \end{split}$$

and

$$\sigma_c(\lambda|\pm\lambda_2^0) = \sigma_c^0(\lambda) + \int_{-\lambda_2^0}^{+\lambda_2^0} G(\lambda-\lambda')\sigma_c(\lambda'|\pm\lambda_2^0),$$

$$\sigma_c^0(\lambda) = \int_{\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \frac{\mathrm{e}^{-|k|/2}}{1 + \mathrm{e}^{|k|}} \mathrm{e}^{ik(\lambda - q)}.$$
 (27)

Here $x_{0,1}$ ($x_{2,3}$) are the scaling dimensions for the case that one electron is emitted from lower-orbital (upper-orbital) band electrons. Note that the scaling dimensions depend on the momentum of the created hole through the phase shifts n_c and d_c . One can also see that both of the scaling dimensions in (26) include the term $\frac{1}{4}$ which comes from level-1 SU(2) CFT for spin excitations in the same orbital. On the other hand, orbital excitation is described by U(1) CFT which is featured by the dressed charge ξ_{Δ} , since level-1 SU(4) CFT is reduced to two level-1 SU(2) CFTs and U(1) CFT in the presence of orbital splitting.

The critical exponent $X_{\beta}(k)$ is shown in Fig. 1, where the momentum is plotted in the unit of inverse lattice spacing 1/a. In Fig. 1(a), the critical exponent is shown for the case of an electron being emitted from the upperorbital band for several choices of the orbital splitting. It is seen that the critical exponent is strongly dependent on the momentum. In the range where the critical exponent becomes close to zero, the divergence singularity is weakened, whereas for larger negative values of the exponent, the singularity becomes stronger. Shown in Fig. 1(b) is the critical exponent when an electron is emitted from the lower-orbital band. In this case also, the exponent is strongly momentum-dependent, and it can change even its sign, which means that divergent power-law singularity is changed into convergent power-law property in some momentum range. We note that when the orbital splitting Δ is larger than a critical value Δ_c , the upper orbital becomes empty without particles. Then the relevant effective theory simply becomes level-1 SU(2) CFT, and the scaling dimension becomes $\frac{1}{4}$ which was previously obtained by Sorella and Parola, [16,19] and Voit. [20]

B. Critical properties for spinon dispersions

We have so far discussed the critical behavior for the holon dispersion. In the photoemission experiments, the large spectral intensity has been observed not only for the holon dispersion but also for the spinon dispersion. In this section we study critical behavior of photoemission spectra around the spinon dispersions. This problem was recently addressed by Voit by using the Luther-Emery model which does not include the effect of orbital degeneracy. [20] His calculation was based on several conjectures for the spectral functions, because even for the Luther-Emery model the exact dynamical correlation functions cannot be obtained. We shall confirm the validity of his conjectures by using the CFT analysis, and also extend his results to the multi-orbital case.

Let us first recall that in the case of $J \to 0$ (or $U \to \infty$ Hubbard model), the spectra on the spinon dispersion is determined by a band edge singularity of holon. [16,21] We shall see, however, that in the case of $J \neq 0$ spinon excitations at the low-energy regime becomes essential, which indeed controls the critical behaviour of spectral functions on the spinon dispersions. In order to observe critical properties of spectra on the spinon dispersions, we should consider a massive holon with the lowest excitation energy (rapidity q=0), which gives the energy shift for the spinon dispersion. Also, as mentioned before, the holon behaves as if it is a mobile impurity, and affects the critical properties of spinons through the phase shifts caused by a final state interaction.

Since the SU(n) spin model has (n-1)-types of spinons (this number corresponds to the rank of the underlying SU(n) Lie algebra), there show up (n-1) spinon dispersions in the low-energy regime. Though it is not easy to perform Fourier transformation of (16) completely, we can write down its asymptotic form around each spinon dispersion, by extending the results in ref. 17 where a metallic electron system was studied. The spectral function $A_{\beta a}(k, w)$ on each spinon dispersion specified by suffix a is given by

$$A_{\beta a}(k,\omega) \sim (\tilde{\omega} - v_a \tilde{k})^{X_{\beta a}},$$
 (28)

where $\tilde{\omega} = \omega - \Delta \epsilon_c(q=0)$ and $\tilde{k} = k - \Delta p_c(q=0)$. One can see that the energy is shifted by the amount of the lowest excitation energy of holon, $\Delta \epsilon_c(q=0)$. We find that the corresponding critical exponents $X_{\beta a}$ are obtained in terms of a specific combination of conformal dimensions.

$$X_{\beta a} = 2\Delta_a^- + \sum_{i \neq a}^{n-1} (2\Delta_i^+ + 2\Delta_i^-) - 1$$
 (29)

for $a=1,\dots,n-1$, where Δ_{α}^{\pm} are conformal dimensions which are obtained in (15). We should notice again that (28) is not the ordinary one-particle Green function of spinons, but indeed includes the effect of a massive holon via the phase shifts.

We first consider the SU(n) symmetric case without orbital splitting. As mentioned above, the critical exponent does not depend on the momentum in this case because of high spin-orbital symmetry of the system, and $X_{\beta a}$ takes -1/n. In the case of SU(2), $X_{\beta a} = -1/2$, which agrees with the value previously obtained. [20] Let us next discuss the effect of orbital splitting by using the two-band model introduced in III A. In the low-frequency regime we are now interested in, $X_{\beta a}$ is independent of the momentum even in the presence of the splitting, so that we show the values of $X_{\beta a}$ as a function of the orbital splitting in Fig. 2. In Figs. 2(a) and 2(b) the critical exponents are shown for the case of one electron being emitted from the upper and the lower band, respectively. Since each band has SU(2) spin symmetry,

 $X_{\beta 1} = X_{\beta 3}$. When the orbital splitting goes to zero, all the exponents approach the same value -1/4 characteristic of SU(4) case. It is seen from Fig. 2(b) that the exponent can change its sign as the increase of orbital splitting, because of the effect of a final state interaction. It is thus seen that either the divergent or convergent power-law singularity emerges on each spinon dispersion, depending on the value of the orbital splitting.

IV. SUMMARY

We have studied the critical properties in photoemission spectra for the Mott insulator with orbital degeneracy. We have calculated the spectral functions and their critical exponents for the supersymmetric multi-orbital t-J model, by combining the Bethe ansatz with finitesize scaling methods in CFT. It has been confirmed that power-law singularities around the massive holon dispersion as well as the (n-1) massless spinon dispersions are governed by the infrared-divergence properties of massless spinons. This is partly in contrast to the results for the $U \to \infty$ Hubbard model in which a singularity around the spinon dispersion reflects the band-edge structure of the holon dispersion. It has been clarified that for the critical behavior in (n-1) spinon dispersions, the specific combination of conformal dimensions determines the corresponding critical exponents, which are generally different from that for the holon dispersion. The effect of the orbital-splitting has been studied, which induces the momentum-dependent critical exponents in the spectral function.

In this paper, we have studied the specific t-J model with supersymmetry (t=J). Nevertheless, the conclusions obtained in the present paper can be directly applied to more general cases $(t \neq J)$. This is because in the problem of the photoemission, we are concerned with the one hole doped in the Mott insulator, so that the change in t is expected to merely modify the kinetic energy of the doped hole. Also, we have not considered the effect of the Hund coupling. This effect may be particularly important to treat the systems with double exchange interaction (or ferromagnetic Kondo lattice systems). This problem is now under consideration.

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- FIG. 1. Momentum-dependent critical exponents $X_{\beta}(k)$ for the holon dispersion: (a) and (b) correspond to the cases when an electron is emitted from the upper- and lower-orbital band.
- FIG. 2. Critical exponents $X_{\beta a}$ for the spinon dispersions: (a) and (b) correspond to the cases when an electron is emitted from the upper- and lower-orbital band. Note that the orbital-splitting is normalized by the exchange coupling J.